SEGMENT ANALYSIS METHODOLOGY

The ability of a stream to maintain an acceptable dissolved oxygen (DO) concentration is an important consideration in determining its capacity to assimilate wastewater discharges. DO is used in the microbial oxidation of organic and certain inorganic matter present in wastewater. Oxygen supplied principally by reaeration from the atmosphere will replace any DO lost through oxidation processes. If, however, the rate of oxygen use exceeds the rate of reaeration, the DO concentration may decrease below minimum allowable standards.

To predict the variation in DO, as well as ammonia concentration in streams, several computer-based mathematical models have been used. The two models presently utilized are the Modified Iowa and the more sophisticated QUAL-II program. Each of these is described later in this chapter. Input data for the models was developed from existing technical information and recent field investigations of selected streams. When sufficient data was not available, conservative assumptions were made that tend to assure a high degree of protection for water quality without imposing unrealistically stringent effluent limitations. Recent water quality sampling has helped to demonstrate the reliability of particular constants and assumptions used and has improved the validity of the models. Available data allows a reasonably accurate prediction of the impact of different wastewater loads or treatment arrangements upon the DO and ammonia concentrations to be performed. The current data also allows for the determination of wastewater discharges that will not result in violation of water quality standards.

THEORY AND METHODOLOGY

Modeling Theory

Dissolved oxygen (DO) concentrations in streams are controlled by many factors including atmospheric reaeration, biochemical oxygen demands (carbonaceous and nitrogenous), algal photosynthesis and respiration, benthal oxygen demands, temperature, and the physical characteristics

of the stream. Many of these factors are difficult, if not impossible, to accurately assess. As a result of this difficulty, limitations on the use of these controlling factors are discussed below.

Photosynthesis can produce large quantities of oxygen during the day if algae are present in the stream. Conversely, at night, algal respiration creates an oxygen demand. Research efforts have attempted to fit harmonic functions to this phenomenon, but with limited success. Specific allowance for diurnal fluctuations in oxygen levels is only included in the QUAL-II computer model.

Benthal oxygen demands result from anaerobic decomposition of settled organic material at the bottom of the stream. These reactions release carbonaceous and nitrogenous organic materials that create biochemical oxygen demands. The inclusion of benthal oxygen demands in the QUAL-II model requires extensive field surveys to determine the real extent of sludge deposits within a stream and coefficients that describe the release into the water. Since the impact is minor in most instances and no data are available to accurately describe sludge deposition areas, no special allowance for benthal oxygen demands is included in the Modified Iowa model formulation. However, QUAL-II has provisions for benthic activities, which need sufficient field data to calibrate and verify the rate constants. If field data are not available, default rate constant values can be used.

A complete mathematical model to describe DO concentrations within the stream would include all significant factors. Natural streams cannot presently be expressed mathematically with absolute certainty, but reasonably accurate predictions can be made through realistic assumptions concerning the reaeration phenomenon and deoxygenation caused by carbonaceous and nitrogenous biochemical oxygen demands (BOD). Specific values obtained in detailed field investigations from other locations, with particular emphasis placed upon data collected in Iowa, provide the only basis for defining ranges of coefficient values being incorporated in the water quality models today. The continued effort towards the collection of water quality data at low flow conditions will aid in defining the above coefficient ranges used in the future.

Nitrogenous BOD is due to the oxidation of ammonia to nitrates by certain species of bacteria. This oxidation process is called nitrification. Nitrification is a two-step process whereby a specific bacterial species oxidizes ammonia to nitrite and a different bacterial species oxidizes the nitrite to nitrate.

Theoretically, approximately 4.5 mg/l of oxygen are required to oxidize 1.0 mg/l of ammonia (expressed as nitrogen) to nitrate. This theoretical value may conservatively over estimate the oxygen demand of nitrification as the nitrifiers obtain oxygen from inorganic carbon sources during combined energy and synthesis reactions. Actual values obtained have varied between 3.8 and 4.5 mg/l of oxygen per mg/l of ammonia nitrogen (NH_3-N). The Modified Iowa model uses 4.33 as the ratio of nitrogenous BOD to NH_3-N. Since secondary wastewater treatment plant effluents quite commonly contain NH_3-N levels of 10 mg/l during summer operations and 15 mg/l during winter periods, the equivalent nitrogenous BOD (should all the ammonia be converted to nitrates) is approximately 40-46 mg/l (summer) and 62-68 mg/l (winter).

Modified Iowa Model

The Modified Iowa model is a minor refinement of computer program used by the Department since 1976 to determine wasteload allocations (WLA). These refinements were recommended by the consulting firm, JRB Associates, McLean, Virginia, as part of the their review of the Department's water quality models. The specific modifications are presented in a User's Manual and described in detail later in this section. The major changes include: replacement of the existing temperature adjustments for nitrification rates, equations to account for algae uptake of ammonia, and a photosynthesis minus respiration (P – R) term for improvement of summer dissolved oxygen (DO) simulation. A copy of the complete user's manual is available from the Department (User's Manual for Modified Iowa DEQ Model, June 1983).

1. Dissolved Oxygen Deficit Equation

The Modified Iowa model uses a version of the Streeter-Phelps equation for DO deficit within the stream. This approach recognizes carbonaceous and nitrogenous BOD, atmospheric reaeration, initial DO deficit, and photosynthesis. The effects of photosynthesis and benthal oxygen demands are not specifically considered. The modified Streeter-Phelps equation suggested for use by JRB Associates is as follows:

$$D(t) = \frac{K_1 L_o}{K_2 - K_1}(e^{-K_1(t)} - e^{-K_2(t)}) + \frac{K_n N_o}{K_2 - K_n}(e^{-K_n(t)} - e^{-K_2(t)}) + D_o e^{-K_2(t)} + \frac{(R-P)}{K_2}(1 - e^{-K_2(t)})$$

where:

$D(t)$ = DO deficit at time t, mg/l
D_o = Initial DO deficit, mg/l
L_o = Initial ultimate carbonaceous BOD concentration, mg/l
N_o = Initial ultimate nitrogenous BOD concentration, mg/l
K_1 = Carbonaceous deoxygenation rate constant, base e, day^{-1}
K_N = Nitrogenous deoxygenation rate constant, base e, day^{-1}
K_2 = Reaeration rate constant, base e, day^{-1}
R = Algal respiration oxygen utilization, mg/l/day
P = Photosynthetic oxygen production, mg/l/day
t = Time of travel through reach, day

In this equation, the rates of oxygen utilization due to carbonaceous and nitrogenous BOD and algal activity are expressed as first order reaction rates. This is an accepted procedure for the carbonaceous demand, but represents a simplification for the nitrogenous demand. The "P – R" term represents the modification to the traditional Streeter-Phelps equations to account for algal influences to the available DO in the stream. The other traditional Streeter-Phelps components (Streeter, 1925) remain unchanged. The "P – R" term was obtained from the MS-ECOL fresh water model (Shindala et al., 1981).

The ultimate carbonaceous and nitrogenous BOD concentrations as a function of time (t) are calculated as follows:

$$L(t) = L_o e^{-K_1(t)}$$

$$N(t) = N_o e^{-K_n(t)}$$

where:

$L(t)$ = Ultimate carbonaceous BOD at time, t, mg/l
$N(t)$ = Ultimate nitrogenous BOD at time, t, mg/l

Since nitrification is a two-step process, many researchers have proposed that it is a second order reaction. However, most water quality models assume that it is a first order reaction for the ease of programming and usage.

Nitrifying bacteria are generally present in relatively small numbers in untreated wastewaters. The growth rate at 20°C is such that the organisms do not exert an appreciable oxygen demand until about eight to ten days have elapsed in laboratory situations. This lag period, however, may be reduced or eliminated in a stream due to a number of reasons including the following: the discharge of large amounts of secondary effluent containing seed organisms, and nitrifier population buildup on the stream's wetted perimeter. In biological treatment systems, substantial nitrification can take place with a resultant build-up of nitrifying organisms. These nitrifiying bacteria can immediately begin to oxidize the ammonia present and exert a significant oxygen demand in a stream below the outfall.

It is known that the biological nitrification process is generally more sensitive to environmental conditions than carbonaceous decomposition. The optimal temperature range for growth and reproduction of nitrifying bacteria is 26° to 30° C. It is generally concluded that the nitrogenous BOD will assume greatest importance in small streams which receive relatively large volumes of secondary wastewater effluents during the low flow, warm weather periods of the year (August and September). These conditions were used for the low flow determination of allowable effluent characteristics during summer periods. During winter low flow periods (January and February), nitrification will probably have limited influence upon the oxygen demand due to the intolerance of nitrifying bacteria to low temperatures. During analysis of winter low flow conditions, limited nitrification was observed.

2. Respiration and Photosynthesis Equation

The equations used to calculate P, the photosynethic oxygen production, and R, the algal respiration oxygen utilization, are:

$$P = \frac{(OP)\ (GP - DP)\ (CHLA)}{AP}$$

where:

OP = mg of oxygen produced by algae/mg of algae
AP = ug of chlorophyll–a/mg of algae
GP = Algal growth rate, day^{-1}
DP = Algal death rate, day^{-1}
CHLA = Chlorophyll–a concentration, $\mu g/l$

and

$$R = 0.025\ CHLA$$

The values of OP, AP, and DP are selected from literature values. Current literature values are presented in Table IV-3 (page 72). It is essential that chlorophyll-a measurements be available from the stream sampling data. If not, chlorophyll-a values must be estimated by general field observation or conditions on a similar stream, which detracts from the credibility of the calibration. Since nitrate and inorganic phosphorus are not included in the model, the growth rate (GP) must be calculated outside the model using the equation:

$$GP = \lambda\ \frac{(N)}{(N + K_{MN})}\ \frac{(P)}{(P + K_{MP})}\ \frac{(LI)}{(LI + K_{LI})}$$

where:

GP = Local algal growth rate at 20°C, day^{-1}
$\rangle$ = Maximum specific algal growth rate at 20°C, day^{-1}
N = Sum of observed instream concentrations of NH_3-N and nitrate
     nitrogen (NO_3-N), mg/l
K_{MN} = Michaelis-Menton half saturation constant for total inorganic N,
       mg/l
P = Observed instream concentration of inorganic phosphorus, mg/l
K_{MP} = Michaelis-Menton half saturation constant for inorganic P, mg/l
LI = Average incident light intensity, $kcal/m^2$-sec
K_{LI} = Michaelis-Menton half-saturation constant for light, $kcal/m^2$-sec

Literature values for ⟩, K_{MN}, K_{MP}, LI, and K_{LI} are shown in Table IV-3 (page 72).

The values of OP and AP are input as constants for the entire stream, while GP, DP, and CHLA are specified for each reach. The Michaelis-Menton constants are used to adjust the maximum potential algal growth rate by the amounts of light, nitrogen, and phosphorus that can limit algal growth. Each Michaelis-Menton constant is the concentration at which that particular constituent limits algal growth to half the maximal or "saturated" value.

3. Algal Uptake of Ammonia Equation

Another new feature in the Modified Iowa model is the simulation of the algal uptake of ammonia nitrogen (NH_3-N). The instream concentrations of inorganic nutrients are reduced by phytoplankton consumption. Phytoplankton requirements for inorganic N may involve both NH_3-N and nitrate nitrogen (NO_3-N). The fraction of consumed nitrogen which is NH3-N must be known if instream concentrations of NH_3-N are to be properly simulated. This fraction is the preferential NH_3 uptake factor.

The amount of NH_3-N removed by algae in a reach is calculated by the following equation taken from the MS-ECOL model (Shindala et al., 1981):

$$UP = \frac{(GP)(ANP)(NF)(CHLA)(e^{(GP-DP)(t)} - e^{-(K_N)(t)})}{(GP - DP + K_N)}$$

where:

UP = Amount of NH_3-N removed in a reach, mg/l
ANP = mg N/ug chlorophyll-a
NF = Fraction of NH_3 preferred for algal uptake (0 – 0.9)
t = Time of travel through reach, day

The model calculates 't' internally. The values of ANP and NF are obtained by calibration or from literature values. Ranges of literature values are found in Table IV-3 (page 72). The model assumes that algal uptake of ammonia occurs until the instream concentration of NH_3-N is equal to the inorganic N half saturation constant K_{MN}. If the instream concentration of NH_3 is below the half-

saturation constant, the technical literature indicates that algae will switch to nitrate (NO_3) as the sole source of nitrogen.

4. Rate Constant Determination

a. Deoxygenation Rate Constants

The carbonaceous deoxygenation rate constant (K_1) for most streams will vary from 0.1 to 0.5 per day (base e, 20 °C). Early work by Streeter and Phelps (Streeter, 1925) determined an average value for the Ohio River of 0.23/day at 20°C (0.1/day, base 10). This value has been accepted and commonly used with reasonable results.

Specific deoxygenation rates for selected Iowa stream segments have been determined from stream surveys performed since 1977. These specific rates showed wide variations within each stream segment and among various streams. Thus, the carbonaceous deoxygenation rate of 0.2/day at 20°C is still used as an initial starting point in calibration/verification efforts. Future stream studies will be used to verify the specific rates applicable for Iowa streams.

Information on nitrogenous deoxygenation rates is extremely limited; however, available information indicates that nitrification rates (when active nitrification does occur) are somewhat greater than carbonaceous oxidation rates. Therefore, the nitrogenous deoxygenation rate (K_N) (0.3/day at 20°C was selected) is used as input data unless calibration/verification efforts provide a more reliable value. Again, future field measurements of typical nitrogenous deoxygenation rates in Iowa streams would greatly enhance the accuracy of the modeling effort.

The modified model alters the value of K_N within each reach as a function of the stream DO concentration. Because nitrifying bacteria are very sensitive to DO levels, K_N is reduced when low DO conditions exist. The following equation, which accounts for the effect of DO concentrations on nitrification rates, is taken from the Wisconsin QUAL III Model (WDNR, 1979):

$$PN = 1 - e^{-(0.52)(DO)}$$

where:

PN = Nitrification reduction factor
DO = Dissolved oxygen concentration, mg/l

The K_N value input to the model is multiplied by the reduction factor PN when DO concentrations are low. The product is the value of K_N, which is used in the DO deficit and nitrogenous BOD equations.

b. Reaeration Rate Constant

The relationship of Tsivoglou and Wallace (Tsivoglou, 1972) was adopted for determination of the reaeration rate constant. This formulation is based on the premise that the reaeration capacity of nontidal fresh water streams is directly related to the energy expended by the flowing water, which in turn is directly related to the change in water surface elevation.

The average rate of energy expenditure is found by dividing the change in water surface elevation by the time of flow. The original Tsivoglou and Wallace formulation has been modified to account for the percentage of ice cover. This relationship is expressed by:

$$K_2 = \frac{c\Delta h \ (ICE)}{t}, \text{ at } 20°C$$

where:

K_2 = Reaeration rate constant, 1/day, base e
c = Gas escape coefficient, 1/ft.
Δh = Change in water surface elevation, ft.
ICE = Factor reflecting effect of ice cover on reaeration rate (unitless)

$$1 - \left(0.95 \times \frac{percent \ ice \ cover}{100} \right)$$

t = Time of travel (days)

Tsivoglou's equation was derived from actual measurement of stream reaeration rates by a field tracer procedure in which a radioactive form of the noble gas krypton served as a tracer for oxygen. In development of Tsivoglou's procedure, other reaeration rate predictive formulas were compared with results obtained from the field tracer technique, but none appeared to predict stream reaeration rates as accurately as the Tsivoglou model.

The calibration results for sampled Iowa streams have indicated that the following guidelines are appropriate with respect to the gas escape coefficient incorporated in the Tsivoglou expression:

$$c = 0.054 \ (@ \ 20°C) \text{ for } 15 \leq Q \leq 3000 \text{ cfs}$$

$$c = 0.115 \ (@ \ 20°C) \ \text{for} \ 0 \le Q \le 15 \ \text{cfs}$$

Other calibrated/verified values may be used on streams with sufficient water quality data.

The ICE factor ranges from 0.05 for complete ice cover to 1.0 for zero cover. The selected input value is based on available field data or estimated by the modeler.

5. Temperature Corrections

Temperature corrections for the carbonaceous and nitrogenous deoxygenation rate constants and the reaeration rate constants are performed within the computer model. The following equations define the specific temperature corrections used in the program:

$$K_{1(T)} = K_{1(20)} \ (1.047^{\ (T-20)})$$
$$K_{2(T)} = K_{2(20)} \ (1.0159^{\ (T-20)})$$
$$K_{N(T)} = K_{N(20)} \ (1.080^{\ (T-20)})$$
$$GP_{(T)} = GP_{(20)} \ (1.047^{\ (T-20)})$$

where:

T = Water temperature, °C

This temperature correction for K_1 represents the state-of-the-art and is a widely accepted formulation. The K_2 and K_N equations represent the more accepted functions used in the Vermont QUAL-II model (Meta Systems, 1979). The growth rate temperature correction is taken from the MS-ECOL model (Shindala et al., 1981).

The principal factor affecting the solubility of oxygen is the water temperature. DO saturation values at various temperatures are calculated as follows:

$$C_s = 24.89 - 0.426T + 0.00373T^2 - 0.0000133T^3$$

where:

T = Water temperature, °F

C_s = Saturation value for oxygen at temperature, T, °F, at standard

pressure

6. Stream Velocity Calculations

Stream velocities are important in determining reaeration rates and the downstream dispersion of pollutants. The computer model calculates velocity based on either a variation of the Manning's Formula for open channel flow or the Leopold-Maddock predictive equation.

a. Manning's Formula

The Manning's Formula for open channel flow is:

$$v = \frac{1.49 R^{2/3} S^{1/2}}{n}$$

> where:
>
> > v = Velocity, fps
> > R = Hydraulic radius, ft
> > S = Channel Slope ft/ft
> > n = Roughness coefficient

For a river or stream with a width much greater than its depth, the value of R is approximately equal to the mean depth. If both sides of the equation are multiplied by the cross-sectional area (width)(mean depth), the following equation results:

$$Q = \frac{1.49}{n} w d^{5/3} S^{1/2}$$

> where:
>
> > d = Mean river depth, ft
> > Q = Discharge, cfs
> > w = Water surface width, ft
> > S = Slope ft/ft
> > n = Roughness coefficient

All variables except for "d" are input values. Internally, the program solves the above equation for d, then calculates the velocity v by:

$$v = Q/A = Q/wd$$

River slopes were obtained from existing stream profiles when available, but usually were taken from USGS topographic maps. Slopes obtained from USGS maps are rather generalized, and more accurate river profiles would greatly improve the accuracy of velocity determinations.

River widths were estimated from information obtained from field observations, flow, and cross-sectional data at each USGS gauging station.

Roughness coefficients are estimated from charts and techniques presented in Chow (Chow, 1965). The value of 0.035 is being used on Iowa streams unless the physical characteristics of the stream are more accurately reproduced by another value.

In developing the particular model run for a stream segment, depth and velocity data from stream gauging stations or from field surveys are used to extrapolate depth and velocity at other points along the segment. The extrapolation is a rough approximation; however, it is reasonably close over the average length of a stream. When available, the uses of field investigations to determine actual stream velocities and depths at many selected stream sites in the modeled segment have improved the accuracy of the model.

The Manning's equation is used where little historical flow and velocity information exists in the stream segment. If flows and velocities are measured during a calibration sampling event, the roughness coefficient "n" can be calibrated. However, in most instances, more reliable flow velocity relationships can be modeled by using the Leopold-Maddock equation.

b. Leopold-Maddock Equation

The Leopold-Maddock (Leopold, 1953) equation predicts stream velocity as a function of discharge according to:

$$V = aQ^b$$

where:

V = Stream velocity, ft/sec
Q = Discharge, cfs
a, b = Empirical constants

It is significant to point out that the empirical constants a and b apply to a specific stream cross section. The value of "b" represents the slope of a logarithmic plot of velocity versus discharge. The value of "a" represents the velocity at a unit discharge.

The Leopold-Maddock equation has been used in many studies and has been found to produce reliable results when the empirical constants are properly evaluated. However, its use is limited to streams for which historical data are not available for determining representative values for the empirical constants. A regression analysis is performed on several sets of velocity-discharge data to determine the empirical constants. The data selected for use in the analysis corresponds to low stream flow conditions since the use of elevated stream flow data may bias the results.

Since reaches of uniform cross section, slope, and roughness parameters rarely characterize stream systems, the empirical constants are determined for several representative cross sections of each stream system to be modeled. The same values of the empirical constants usually do not apply to all reaches along a stream segment unless field measured data indicates otherwise. JRB Associates staff indicated that a value for "b" of 0.25 is commonly used for smaller streams and rivers, such as those found in Iowa. Thus, where limited field information exists, "a" can be determined if "b" is assumed to equal 0.25 by solving the above equation. This assumption will only be used if there is insufficient flow or stream cross sectional data. Velocity and discharge values can be obtained from the USGS gauging station data forms 9-207 or from stream surveys obtaining current meter and cross section measurements.

7. Computer Input and Output Data

In order to calculate water quality at various points in the river, the river length to be modeled is divided into reaches. River characteristics (mean widths, depths, velocities, deoxygenation and reaeration rate constants, and water temperatures) were considered for each small reach. The overall stream length modeled should be less than 20 miles to insure steady state conditions.

One or more of the following set the location of the reaches:

a. A tributary.

b. A wastewater discharge.

c. A change in river characteristics, such as river width or slope.

d. A dam.

In order to calculate water quality characteristics at various points within each reach, the reaches are divided into segments called sections.

Actual data input into the computer program are as follows:

1. Initial river conditions such as flow and concentration of ultimate carbonaceous BOD, ammonia nitrogen (NH_3-N), and Dissolved Oxygen (DO).

2. Uniform background flow contributions for each reach and concentrations of ultimate carbonaceous BOD, NH3-N, and DO in the groundwater.

3. The number of reaches.

4. For each reach the following:

    a. Length

    b. Number of sections

    c. Water temperature

    d. Channel slope

    e. River width ———— used in Tsivoglou & Manning equations

    f. Roughness coefficient

    g. Deoxygenation rate constants

    h. Empirical constants – Leopold-Maddock equation

    i. Ice cover

5. Wastewater or tributary inflows consist of inflow rates, ultimate carbonaceous BOD, NH_3-N, and DO concentrations.
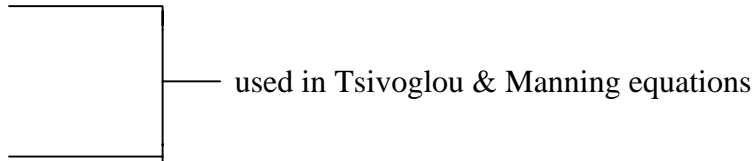
The computer printout of the model run includes a reformat of all input data and key calculated data for each stream reach and segment.

This calculated data includes:

1. Stream velocity

2. Rate constants

3. Saturated DO concentration

4. Travel time

5. BOD_u, NH_3-N and DO instream concentrations

An example of the output is found in the <u>User's Manual for Modified Iowa DEQ Model.</u>

TABLE IV-3
TYPICAL VALUES OF INPUT VARIABLES
FOR MODIFIED IOWA MODEL

VARIABLE	DESCRIPTION	RANGE OF VALUES	RECOMMENDED WLA VALUE
NF	Preferential NH_3 uptake factor	0 – 0.9	Calibrate
ANP	mg Nitrogen/ug Chlorophyll-a	0.0007 – 0.009	Calibrate
K_{MN}	Michaelis-Menton half-saturation constant for nitrogen (mg/l)	0.01 – 0.20	Calibrate
K_{MP}	Michaelis-Menton half-saturation constant for phosphorus (mg/l)	0.01 – 0.05	Calibrate
K_{LI}	Michaelis-Menton half-saturation constant for light (mg/l)	--------	0.0035
AP	ug Chlorophyll-a/mg Algae	10 - 100	Calibrate
OP	mg Oxygen produced by Algae/mg Algae	1.4 – 1.8	1.63
K_1	Carbonaceous deoxygenation rate constant (day^{-1})	0.02 – 3.4	Calibrate
K_N	Nitrogenous deoxygenation rate constant (day^{-1})	0.3 – 3.0	Calibrate
C	Tsivoglou escape coefficient (ft^{-1})	--------	0.054, $15 \leq Q \leq 3000$ cfs 0.110, $1 \leq Q \leq 15$ cfs
$\rangle$	Maximum algal growth rate (day^{-1})	1 - 3	2
DP	Local algal death rate (day^{-1})	0.024, 0.24	Use higher value if nutrients are scarce or chlorophyll-a concentration exceeds 50 µg/l; otherwise use lower value
ICE	Factor relating ice cover to reduced reaeration capacity	0.05 – 1.0	Field observation

Vermont QUAL-II Model

The Vermont QUAL-II water quality model can simulate conservative and nonconservative constituents in branching stream and river systems. The constituents that can be modeled by the revised version of QUAL-II are:

- Dissolved Oxygen (DO)
- Biochemical Oxygen Demand (BOD)
- Temperature
- Algae
- Organic Nitrogen
- Ammonia Nitrogen (NH_3-N)
- Nitrite (NO_2-N)
- Nitrate (NO_3-N)
- Dissolved Phosphorus
- Organic Phosphorus
- Coliform
- Conservative Substances

The model was adapted for Iowa conditions and needs by JRB Associates. A copy of the detailed User's Manual can be obtained from the Department ("User's Manual for Vermont QUAL-II Model", June 1983). The User's Manual will provide documentation of the theoretical aspects of the model as well as a description of the model input and data requirements. The following discussion is, in part, key items from the User's Manual. The size
and complexity of the document prohibits its reproduction in this chapter of the "Basin Plan Support Document".

1. Background

The QUAL-II model is an extension of the stream model, QUAL-I, developed by F.D. Masch and Associates and the Texas Water Development Board in 1971. QUAL-I was originally designed to simulate the dynamic behavior of conservative materials, temperature, BOD, and DO in streams.

Water Resources Engineers, Inc. (WRE) revised the QUAL-I model to include the steady state simulation of NH_3, NO_2, NO_3, dissolved phosphorus, algae, and coliforms as well as DO and BOD. This WRE QUAL-II model has since undergone numerous revisions to incorporate additional parameters and changes in constituent interactions. The version of QUAL-II that is used by the Department is the Vermont version of QUAL-II.

The Vermont QUAL-II is basically a version developed by Meta Systems, Inc. (1979), with later modifications by Walker (1980, 1981) and the Vermont Department of Water Resources and Environmental Engineering (1981). The changes Meta Systems introduced in 1979 to U.S. EPA's version of QUAL-II include the following:

- Incorporation of the simulation of organic nitrogen.
- Provision of algal uptake of ammonia as a nitrogen source.
- Steady state calculation of diurnal oxygen variations due to algal photosynthesis and respiration based on diel curve analysis.
- Changes in the model to delete the dynamic simulation of DO, thus allowing dynamic simulation of temperature only.
- Inclusion of dam reaeration.
- Changes in the methods used to calculate the reaeration coefficient, K_2.
- Deletion of the radionuclide simulation.

Vermont later added this simulation of organic phosphorus and has modified the expressions for algal kinetics to the QUAL-II version developed by Meta Systems, Inc. (1979).[2]

2. Stream System Representation

QUAL-II permits any branching, well-mixed stream system to be modeled. It assumes that the major transport mechanisms, advection and dispersion, are significant only along the longitudinal axis of the stream. It can handle multiple waste discharges, withdrawals, tributary flows, incremental inflow, flow augmentation, and dam reaeration. Hydraulically, QUAL-II is limited to the simulation of time periods during which the stream flows in the river basin are essentially constant (Roesner, et al., 1981). Thus, the length of river or stream to be modeled is

relatively short, less than 20 miles. The length should be long enough to account for the decay of organic pollutants and the recovery to near background conditions. The use of this model is not suitable for one run over the entire stream or river length.

Streams to be simulated by QUAL-II are divided into reaches, and further subdivided into computational elements. River reaches are the basis of most data input. Hydraulic data, reaction rate coefficients, initial conditions, and incremental inflow data are constant for all computational elements within a reach. For the purposes of QUAL-II, the stream is

_____

[2] The majority of the information in the User's Manual came from the following four sources:
   Meta Systems, Inc. Documentation for the Meta Systems Version of the QUAL-II Water Quality
       Simulation Model. July 1979.
   Roesner, L.A., P.R. Giguere, and D.E. Evenson. Computer Program Documentation for Stream Quality
       Modeling (QUAL-II). EPA-600/9-81-014. Athens: U.S. EPA Center for Water Quality Modeling,
       Environmental Research Laboratory, February 1981.
   Roesner, L.A., et al. User's Manual for Stream Quality Model (QUAL-II). EPA-600/9-81-015. February
       1981.
   State of Vermont, Agency of Environmental Conservation, Department of Water Resources and Environmental
       Engineering. Lower Winooski River Wasteload Allocation Study, Part B: Mathematical   Modeling Report.
       January 1982.

conceptualized as a network of completely mixed reactors – computational elements – that are linked sequentially to each other via the mechanisms of transport and dispersion (Roesner, et al., 1981).

Streams to be simulated by QUAL-II are divided into reaches, and further subdivided into computational elements. River reaches are the basis of most data input. Hydraulic data, reaction rate coefficients, initial conditions, and incremental inflow data are constant for all computational elements within a reach. For the purposes of QUAL-II, the stream is conceptualized as a network of completely

mixed reactors – computational elements – that are linked sequentially to each other via the mechanisms of transport and dispersion (Roesner, et al., 1981).

Although QUAL-II has been developed as a relatively general program, Roesner, et al. (1981) cites certain dimensional limitations, which have been imposed upon it during program development. These limitations are as follows:

> Reaches: a maximum of 75
> Computational elements: no more than 20 per reach nor 500 in total
> Headwater elements: a maximum of 15
> Junction elements: a maximum of 15
> Input and withdrawal elements: a maximum of 90 in total

QUAL-II makes certain assumptions about the stream system being simulated, including the following:

- QUAL-II assumes first order kinetics.
- The model utilizes a simplified nutrient-algal cycle with Michaelis-Menton kinetics.
- Only constant inflows and point source discharges are considered in the model.
- Each computational element is assumed to be completely mixed.
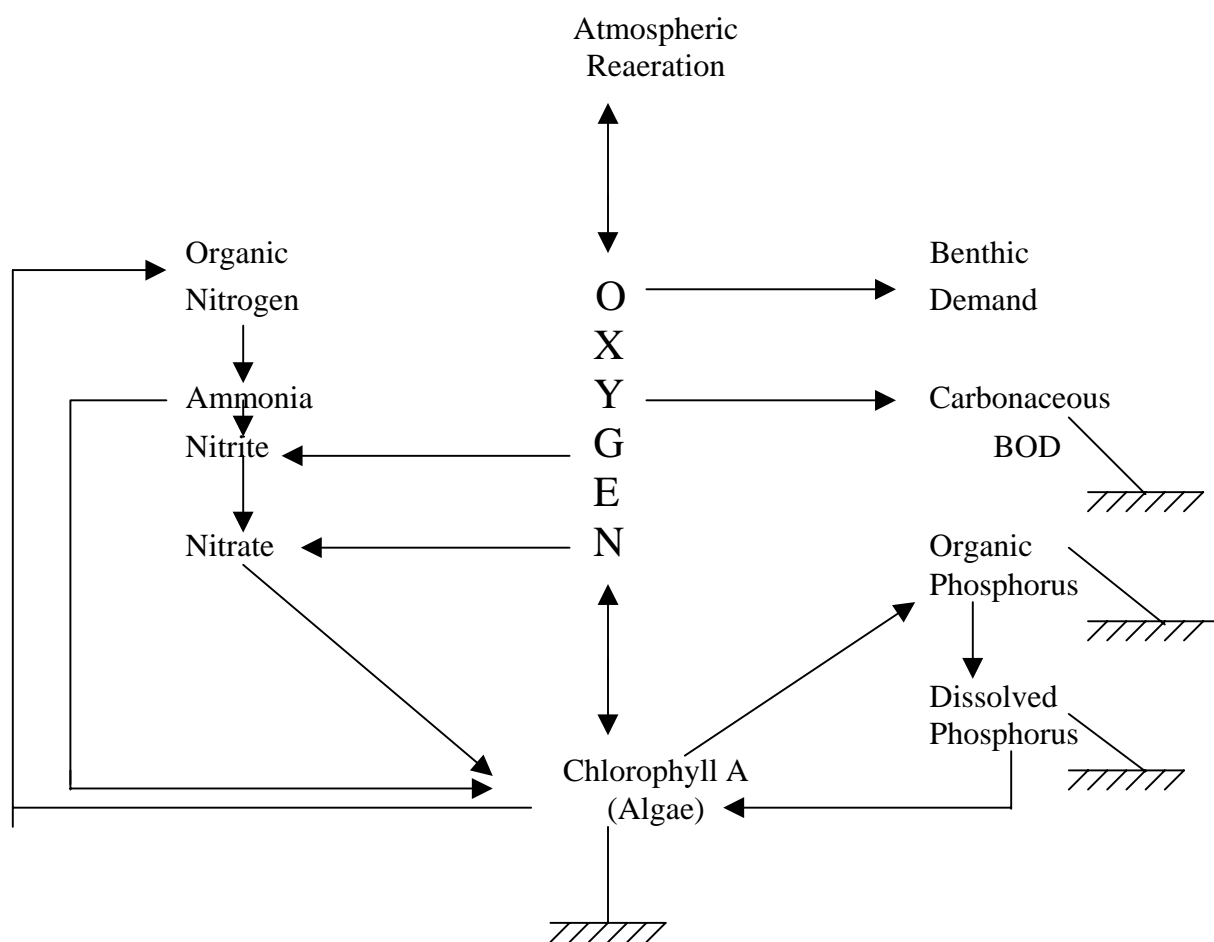- The model does not take into account variations in depth or within stream cross section in each reach.

3. General Model Relationships

QUAL-II utilizes a mass balance differential equation that describes the behavior of a water quality constituent in one dimension. The model is structured to simulate the major interactions of the nutrient cycles, algal production, benthic oxygen demand, carbonaceous oxygen uptake, atmospheric reaeration, and the effect these processes have on receiving water concentrations of dissolved oxygen (DO). The interactions of all these constituents are illustrated in Figure IV-1. Arrows on Figure IV-1 indicate the direction of normal system progression in a moderately polluted environment; the directions may be reversed in some circumstances for some constituents. An example of process reversal: under normal conditions, oxygen will be transferred from the atmosphere into the water. Under conditions of oxygen supersaturation, which can occur as a result of algal photosynthesis, oxygen might actually be driven from solution, causing the direction of flow to reverse (Roesner, et al., 1981).

Coliforms are modeled as nonconservative decaying constituents, and do not interact with other constituents. The conservative constituents, of course, neither decay nor interact in any way with other constituents.

The detailed mathematical relationships that describe the individual reactions and interactions are presented in the User's Manual. Their inclusions would make this document very lengthy and cumbersome. A brief discussion on the mathematical relationships for phytoplanktonic algae is included, as this is one of the significant improvements over the past available model.

Figure IV-1
General Model Structure for QUAL-II

Atmospheric
Reaeration

Organic
Nitrogen

Ammonia

Nitrite

Nitrate

O
X
Y
G
E
N

Benthic
Demand

Carbonaceous

BOD

Organic
Phosphorus

Dissolved
Phosphorus

Chlorophyll A
(Algae)

Source: Vermont, 1982

The chlorophyll-a concentration in a stream system is assumed to be directly proportional to the concentration of phytoplanktonic algal biomass. In QUAL-II, algal biomass is converted to chlorophyll-a by the simple relationship:

$$Chl\text{-}a = a_o A$$

where:

Chl-a = Chlorophyll-a concentration, $\mu g/l$
A = Algal biomass concentration, mg/l
a_o = A conversion factor – chlorophyll-a to algae ratio

The growth of algae (chlorophyll-a) is calculated according to the following differential equation:

$$\frac{dA}{dt} = uA - p_o A - \frac{s}{d}(A)$$

where:

A = Algal biomass concentration, mg/l
t = Time, day
u = The local specific growth rate of algae which is temperature dependent, 1/day
p_o = Algal death rate, 1/day
s = The local settling rate for algae, ft/day
d = Average depth, ft

It should be noted that the local algal growth rate is limited by light and either nitrogen or phosphorus, but not both. Thus, nutrient/light effects are multiplicative but nutrient/nutrient effects are alternate (Walker, 1981). The specific expression used to calculate local algal growth rates are listed in the User's Manual. In the QUAL-II model, the "algal respiration rate" controls only the uptake of oxygen by algae, while the "algal death rate" governs both the change in algal biomass due to endogenous respiration and the conversion of algal P to organic P. The "algal N to organic N" term represents the conversion of algal N to organic N. Algae are assumed to use ammonia and/or nitrate as a source of nitrogen. The effective concentration of available nitrogen is the sum of both concentrations. The algal growth rate and death rates are temperature dependent. They are corrected within the model, as are all other temperature dependent system variables, according to the procedure explained in the User's Manual.

4. Input Data

The first step in setting up the input data for QUAL-II is to prepare a graphic representation of the stream system, similar to that shown in Figure IV-2 (page 81). The best way to begin this is to locate the sampling stations, point source discharges, and stream junctions on USGS topographic maps. Stream miles can then be computed using a map wheel.

As shown in FigureIV-2 (page 81), the stream must be divided into reaches. Reaches are stretches of a stream that exhibit uniform hydraulic characteristics. The reaches are themselves divided into computational elements, which must be the same length throughout the stream system. The length chosen for the computational elements is determined by the degree of resolution needed to approximate the processes taking place in the stream. For example, if the observed dissolved oxygen (DO) concentration goes from saturated concentration to critical concentration and back to saturated concentration over an interval of about five river miles, a degree of resolution of less than one mile is appropriate (Roesner, et al., 1981).

A sketch should be made of the stream reach configuration and the elements numbered. Each computational element is numbered sequentially, beginning with the uppermost point of the stream and proceeding downstream. When a junction is reached, the numbering scheme proceeds from the main stream element immediately upstream of the junction, to the uppermost point of the tributary, and continues downstream. Figure IV-2 (page 81) illustrates this numbering sequence.

Figure IV-2
Sample Reach Network
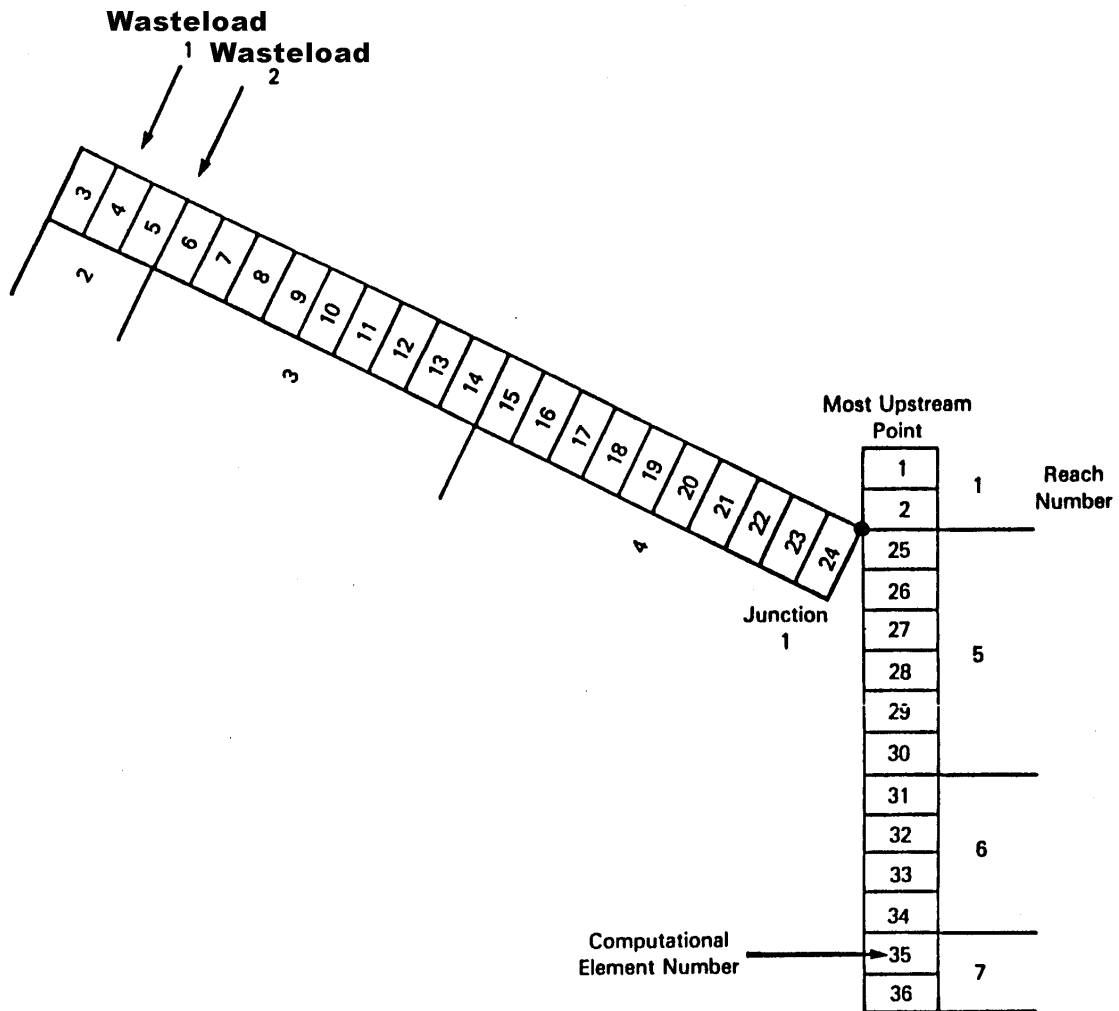
Each computational element in the stream reach network is classified into element types. These element types provide the location of discharges, withdrawls, tributaries, etc. The seven element types used in QUAL-II are:

Number	Type
1	Headwater source element
2	Standard element, incremental inflow only
3	Element on main stream immediately upstream of a junction
4	Junction element
5	Most downstream element
6	Input element
7	Withdrawal element

Special attention should be paid to the numbering of elements, particularly at the junctions. The point source loads are numbered downstream in the order of the elements. Any withdrawls are counted as a point source load in the numbering scheme. It is important that this be done correctly, since QUAL-II associates the first wasteload card with the first type 6 or 7 element in the stream configuration. The same is true of the order of the headwaters.

For informational purposes, the following types of input data groups show the complexity and flexibility of the QUAL-II program. These 12 groups each contain different categories of information that the user must supply to the program.

Card Type 0	Titles
Card Type 1	Control Data
Card Type 1A	Model Parameters
Card Type 2	Reach Identification
Card Type 3	Flow Augmentation Data
Card Type 4	Computational Element Flag Fields
Card Type 5	Hydraulic Data
Card Type 6	BOD and DO Reaction Rates
Card Type 6A	Algae, N, and P Constants
Card Type 6B	Other Coefficients
Card Type 7	Initial Conditions
Card Type 7A	Initial Conditions (continued)
Card Type 8	Incremental Runoff Conditions

Card Type 8A   Incremental Runoff Conditions (continued)
Card Type 9   Stream Junction Data
Card Type 10   Headwater Sources
Card Type 10A   Headwater Sources (continued)
Card Type 11   Point Source Inputs and Withdrawals
Card Type 11A   Point Source Inputs and Withdrawals (continued)
Card Type 12   Dam Reaeration Data

Specific input sequences and formats are presented in the User's Manual. Detailed procedures for calibrating the rate constants to specific stream conditions are also presented in the User's Manual. While running the program for a specific stream or for calibrating a segment, the suggested ranges for reaction coefficients are presented in Table IV-4 (pages 84-85). These values serve as a guide for a run of the QUAL-II program. Since the QUAL-II program is written in FORTRAN, it is essential that the input data be in the correct format for the program to run.

TABLE IV-4
RECOMMENDED RANGES FOR REACTION COEFFICIENTS
FOR QUAL-II

DESCRIPTION	UNITS	RANGE OF VALUES
Ratio of chlorophyll-a to algae biomass	ug Chl-a/Mg A	10 - 100
Fraction of algae biomass that is nitrogen	Mg N/Mg A	0.07 – 0.09
Fraction of algae biomass that is phosphorus	Mg P/Mg A	0.01 – 0.02
O_2 Production per unit of algal growth	Mg O/Mg A	1.4 – 1.8
O_2 Uptake per unit of algae respired	Mg O/Mg A	1.6 – 2.3
O_2 Uptake per unit of NH_3 oxidation	Mg O/Mg N	3.0 – 4.0
O_2 Uptake per unit of NO_2 oxidation	Mg O/Mg N	1.0 – 1.14
Rate constant for the biological oxidation of NH_3 to NO_2	1/Day	0.10 – 1.00
Rate constant for the biological oxidation of NO_2 to NO_3	1/Day	0.20 – 2.00
Rate constant for the hydrolysis of organic-N to ammonia	1/Day	0.02 – 0.4
Dissolved phosphorus removal rate	1/Day	0.02 – 0.4
Organic phosphorus settling rate	1/Day	0.001 – 0.10
Algal settling rate	ft/Day	0.5 – 6.0
Benthos source rate for phosphorus	Mg P/day-ft	Highly Variable
Benthos source rate for NH_3	Mg N/day-ft	Highly Variable
Organic P decay rate	1/Day	0.1 – 0.7
Carbonaceous deoxygeneration rate constant	1/Day	0.02 – 3.4
Reaeration rate constant	1/Day	0.0 - 100

RECOMMENDED RANGES FOR REACTION COEFFICIENTS
FOR QUAL-II
- Continued -

DESCRIPTION	UNITS	RANGE OF VALUES
Rate of loss of CBOD due to settling	1/Day	-0.36 to 0.36
Benthic oxygen uptake	Mg O/day-ft	Highly Variable
Coliform die-off rate	1/Day	0.5 – 4.0
Maximum algal growth rate	1/Day	1.0 – 3.0
Algal death rate	1/Day	0.024 – 0.24
Preferential NH_3 uptake factor	--------	0.0 – 0.9
Algal N to organic N decay rate	1/Day	0.11
Algal respiration rate	1/Day	0.05 – 0.5
Michaelis-Menton half-saturation constant for light	Langleys/min	0.02 – 0.10
Michaelis-Menton half-saturation constant for nitrogen	mg/l	0.01 – 0.20
Michaelis-Menton half-saturation constant for phosphorus	mg/l	0.01 – 0.05
Non-algal light extinction coefficient	1/ft	Variable
Algal light extinction coefficient	(1/ft)/(ug Chl-a/L)	0.005 – 0.02

MODELING DATA SOURCES

The bulk of the work in stream water quality modeling is the collection and interpretation of all available data describing the stream system to be modeled. This section describes procedures and data sources that may be used in stream modeling for wasteload allocations.

Wastewater Discharges

The required data for each discharger consists of effluent flow rates and effluent characteristics such as Biochemical Oxygen Demand (BOD), ammonia nitrogen (NH_3-N), Dissolved Oxygen (DO) concentrations, and temperature. The specific location and characteristics of some smaller wastewater discharges are often unknown and are determined from field investigations or during special stream surveys. Most wastewater discharge information is available in the departmental files.

River Miles

The first step in modeling a river system is determining the locations of all tributaries, wastewater dischargers, dams and other critical points along the river. The total length of the main channel of the river to be modeled must be established and river miles need to be located such that the location of tributaries, etc., can be determined to the nearest one-tenth of a mile. Often the U.S.G.S. or Corps of Engineers has located river miles on larger streams, but in some instances these river miles are incorrect or do not correspond to the existing stream channel. Experience has shown that it is best to start from the beginning with the best available base map and establish river miles by use of appropriate measuring techniques. The best maps to start with are U.S.G.S. topographic maps. These consist of section maps (scale: 1:250,000) and quadrangle maps (scale: 1:24,000). Other maps such as state and county road maps can also be used to supplement the U.S.G.S. maps.

<u>Field Reconnaissance</u>

The following data can be collected during special stream surveys:

1. The precise location of wastewater discharges.

2. The location, condition, height, and type of dams and the nature and approximate length of the pool created by the dam.

3. Approximate river widths at bridge crossings.

4. Approximate shape of channel cross sections.

5. Channel characteristics that will aid in determining the channel roughness coefficients.

The special stream survey should be performed, if possible, during flow conditions that represent the flows used in the modeling effort. Stream discharge information during stream surveys may be verified from data obtained from the U.S.G.S. The stream flow observed during stream surveys is often greater than the $7Q_{10}$. Data such as river widths need to be extrapolated downward to represent $7Q_{10}$ conditions. Shapes of channel cross sections are an aid in this determination.

<u>River Channel Slopes</u>

After river miles and locations are established, the next step is the determination of river channel slopes. During low flow conditions it can be assumed that river channel slopes are essentially the same as the slope of the water surface. Channel profiles can be used as representative of water surface slopes. In some cases, profiles of the river have already been determined. The U.S. Army Corps of Engineers usually does this as part of the work conducted prior to proposal or construction of flood control reservoirs. Without accurate profiles, river slopes can be determined from U.S.G.S. contour maps by locating the points where contour lines cross the river. Stream slopes that are calculated from contour maps only represent an average value over the distance of the river between contour intervals. U.S.G.S. quadrangle maps (if available) are a more reliable source of slope data. Often, these are the only sources available and are the best method of slope determination without an extensive field survey.

River Widths and Roughness Coefficients

River widths and roughness coefficients can be estimated during the field reconnaissance. Roughness coefficients can also be estimated using charts and techniques in hydraulic texts and handbooks. For further discussion, use Open-Channel Hydraulics by Chow, published by McGraw-Hill.

The variation of river widths with discharges can often be determined from data at U.S.G.S. gauging stations. The U.S.G.S. periodically calibrates each gauge. The results from these calibrations are available on U.S.G.S. form 9-207 and include widths, cross-sectional area, mean velocities, and discharges. Reasonably accurate estimations of river widths at the desired discharge can usually be made with this gauging station information along the river widths measured during special stream surveys.

Stream Flow

In the determination of flow conditions throughout the river system to be modeled, all available data from U.S.G.S. flow measuring stations as well as flow rates from all of the wastewater discharges must be obtained. River flows need to be allocated among tributary, groundwater, and wastewater inflow sources. The design low flow is used as the modeling basis, and is determined from a statistical analysis of the flow records at each of the gauging stations in the river system. Design low flows have already been determined for partial and continuous gauging stations (i.e. Iowa Natural Resources Council, Annual and Seasonal Low-Flow Characteristics of Iowa Streams, Bulletin No. 13, 1979). The design low flows at gauging stations must then be allocated to tributaries based on drainage areas. Tributary drainage areas may be available from existing publications (i.e. Larimer, O.J., Drainage Areas of Iowa Streams, Iowa Highway Research Bulletin No. 7, 1957) or they can be determined from U.S.G.S. contour maps.

A summation of tributary inflows and wastewater discharges often is less than the gauged flow. The difference is usually distributed along the main channel of the river as a uniform inflow in terms of cfs per mile of river reach length. If the gauged flow is less than the summation of tributary and wastewater inflows then it is possible to allot a uniform outflow from the main river channel.

Tributary and Groundwater Quality

Values for BOD, NH_3-N, and DO of tributary and groundwater inflow are required for stream modeling. Often, a main tributary to the stream being modeled has also been modeled. In this case, the water quality of the tributary just before discharge into the main stream (as determined by the model) is used. If the tributary is small and has several wastewater discharges, hand calculations can be done to determine its water quality just before entering the main stream.

If the tributary is free of continuous discharging wastewater facilities, water quality has been assumed to be good. The tributary water quality input values are: ultimate BOD – 6 mg/l; NH_3-N concentrations – 0.0 mg/l (summer), 0.5 mg/l (fall, winter, and spring); and DO at saturation.

Groundwater is also noted to be of high quality. The model input values for groundwater are ultimate BOD of 6 mg/l and NH_3-N at 0 mg/l. Groundwater DO's may be quite low depending on how it enters the stream. If it is subsurface flow, DO may be close to zero. A groundwater DO of 2 mg/l is used in wasteload allocation (WLA) work in Iowa.

Rate Constants

The reaeration rate constant (K_2) is usually determined from one of many available predictive formulas. The constant primarily used by the Department is based on Tsivoglou's formula.

Carbonaceous and nitrogenous deoxygenation rate constants are best determined experimentally for a specific wastewater effluent and/or calibrated for a specific stream. However, when specific values are not available, "typical" values from similar streams may be used. In most cases the carbonaceous deoxygenation rate constant (K_1) will not be less than 0.2 per day (20°C). Values as high as 3.4 per day (20°C) have been reported in the literature.

Less information is available on the nitrogenous deoxygenation rate constants or nitrification rates in streams. Experimental work in Illinois (State of Illinois, Environmental Protection Agency, Guidelines for Granting of Exemptions from Rule 404(C) and 404(F) Effluent Standards, Oct., 1974) determined that the nitrogenous deoxygenation rate constant (K_N) ranged from 0.25 to 0.37 per day with an average value of 0.29 per day at 20°C. The current model uses a K_N value based on stream calibration from the modeled stream or similar streams. Other rate constants for benthic and algal

kinetics are based on calibration data or literature values. Specific explanations of these rate constants are in the User's Manual for the Modified Iowa and QUAL-II models.

Dams and Impoundments

The damming of a stream creates special conditions for water quality modeling. For modeling purposes, dams and the resulting impoundments can be put into one of two classifications.

1. Large dams that back up rather extensive impoundments. Flow through the impoundment is not "plug flow" and inflow may be dispersed in a variety of vertical and horizontal directions.

2. Low-head dams which essentially make the river channel wider and deeper for a maximum distance of several miles. Flow through the impoundment is primarily "plug flow."

Class 1 dams and impoundments cannot easily be modeled to predict water quality. The modeling effort should be stopped at the beginning of the impoundment and started again below the dam. Water quality below the dam can be estimated from knowledge of the size of the impoundment, the method of water withdrawal, and water quality data from stream surveys. Water taken from the lower levels of an impoundment during periods of summer stratification may be low in DO. If water flows over a spillway or an overflow weir it may be close to the DO saturation point. One can expect the BOD and NH_3-N concentrations in the discharge from large impoundments to be low unless the impoundment is highly eutrophic.

Class 2 dams and impoundments can be modeled by treating the impoundment as an enlarged or slower moving reach of the river. The length of the pool backed up by the dam may be divided into one or more reaches. Widths can be approximated from field observations. Slopes are taken as the water surface elevation and are quite small, generally elevation drops off no more than a foot over the length of the pool.

The dams may be treated as a reach 0.001 miles or 5.28 feet in length. The slope of this reach then becomes the dam height divided by 5.28 feet. The only water quality parameter that is significantly affected through the dam reach is the DO. Tsivoglou's reaeration rate constant prediction formula can be used to quite effectively predict reaeration over a dam. The equation for change in the DO deficit with time is:

$$D_t = D_o e^{-K_2 t}$$

where:

D_t = DO deficit at time, t
D_o = DO deficit at time zero
K_2 = Reaeration rate constant

Tsivoglou's reaeration rate constant predictive equation (neglecting ice conditions) is:

$$K_2 = \frac{c \Delta H}{t}$$

where:

c = Escape coefficient
ΔH = Change in elevation in time, t

Substituting into the DO deficit equation one obtains:

$$D_t = D_o e^{-c \Delta H}$$

<u>Example:</u>

With a dam 10 feet high and $c = 0.115/ft$. the ratio of D_t/D_o is 0.32 or the deficit is 32 percent of the deficit at time zero. This is a DO deficit recovery of 68 percent.

<u>Winter Conditions Significance</u>

Often the most critical period for maintaining water quality standards is during the winter design low flow periods instead of the summer period. Rates of deoxygenation are greatly reduced at the low temperatures, but ice cover also greatly reduces reaeration resulting in DO levels that may be critical. Nitrification is significantly reduced at freezing temperatures. Consequently, ammonia concentrations may remain elevated over long stream reaches. Some loss of ammonia may occur in stream reaches due to algal uptake.

During winter periods reaeration rates may need to be reduced in proportion to the extent of ice cover. Even with 100 percent ice cover a small amount of reaeration undoubtedly takes place. In the WLAs, reaeration rates were reduced in direct proportion to the estimated ice cover. The ice cover factor is assumed to vary in relationship with the amount of heated water in the discharge. The values range from 95% ice cover to 0% ice cover over dams. Research and field investigations are needed on the effects of ice cover on stream reaeration rates and the extent of ice cover on specific stream reaches in order to more precisely define the applicable reduction factor.